

Fermi arcs and isotope effect of the magnetic penetration depth in underdoped cuprates

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Abstract. - The isotope coefficient β of the magnetic penetration depth in the superconducting state is studied at $T = 0$ for a d -CDW and a nodal metal model. Disregarding superconductivity the Fermi surface of the first model possesses arcs whereas the second model has no arcs. We show that a large increase of β in the pseudogap region is generically incompatible with Fermi arcs in the pseudogap state. Thus only the second model shows a large increase of β with decreasing doping. The required electron-phonon coupling is small and compatible with first-principles calculations based on the local density approximation (LDA).

Underdoped high- T_c cuprates show properties which are not expected to occur in Fermi liquids. [1] There is an energy gaplike feature (pseudogap) seen already well above the transition temperature T_c which increases with decreasing doping. At the same time the large Fermi surface of the normal state at large dopings transforms in the underdoped region into arcs around the nodal direction and becomes gapped near the antinodal points. [2] The temperature dependence of the length of these Fermi arcs is presently controversially discussed. In particular, it is debated whether for $T \rightarrow 0$ and in the absence of superconductivity their lengths would approach zero [3] or a finite value. [4]

Another unexpected feature of underdoped cuprates is the observed large isotope effect β for the magnetic penetration depth. β is very small in the overdoped region, increases strongly with decreasing doping, and may then reach values of the order of one. [5, 6] Such large values cannot be explained by Eliashberg theory where β is practically zero in agreement with a recent experiment in the strong-coupling superconductor MgB_2 [7].

The aim of this Letter is to show the strong interrelation between the pseudogap and Fermi arcs at $T=0$ and β in the underdoped regime. Anomalously large isotope coefficients due to the presence of the pseudogap have been sug-

gested previously. [8] For the coefficient α , describing the change in T_c due to isotope substitution, detailed quantitative calculations [9, 10] yielded large enhancements of α even for a small electron-phonon (EP) coupling due to the presence of a pseudogap in rough agreement with the experiments. Similar calculations for β , presented in this Letter, yield a more complex picture. An enhancement of β does not only require a pseudogap but it is generally incompatible with Fermi arcs at $T = 0$ formed by infinitely sharp quasiparticles. To show this we first study a d -CDW model which can be derived from the t - J model within mean field theory. Such a model is generic for models where the pseudogap is associated with long-range order in the particle-hole channel yielding Fermi arcs at $T = 0$ due to imperfect nesting. We show that this model leads to negligible values for β in the underdoped region because some integrals perpendicular to the arcs diverge if the superconducting gap tends to zero. One way to avoid these divergencies is provided by the nodal metal model which has no arcs. Explicit calculations show in this case indeed a large increases of β and a ratio of β/α of about 2 in the underdoped region in agreement with experiment.

Our calculation is based on the large N limit of the t - J model (N is the number of spin components) [11] which represents a model with competing d -CDW and d -wave su-

perconducting order parameters. [12] For calculating β we add as in Ref. [10] a phonon-induced interaction $V(\mathbf{k} - \mathbf{k}')$ between electrons. In the following only the d -wave part of V is required which is obtained by replacing $V(\mathbf{k} - \mathbf{k}')$ by $4V\gamma(\mathbf{k})\gamma(\mathbf{k}')$ which defines the d -wave coupling constant V for a phonon-induced nearest neighbor interaction. $\gamma(\mathbf{k})$ is equal to $(\cos(k_x) - \cos(k_y))/2$.

The isotope coefficient β for the phase stiffness Λ is defined by $\beta = \frac{1}{2} \frac{\partial \ln \Lambda}{\partial \ln \omega_D}$. Λ is related to the magnetic penetration depth λ by $\Lambda = c^2/(4\pi e^2 \lambda^2)$ where c and e are the velocity of light and the electronic charge, respectively. ω_D is the Debye frequency which is assumed to be proportional to $M^{-0.5}$ where M is the ionic mass. At zero temperature only the diamagnetic term contributes to Λ in the superconducting state which is given by

$$\Lambda = \frac{1}{N_c} \sum_{\mathbf{k}, \alpha} n_{\alpha}(\mathbf{k}) \frac{\partial^2 \chi_{\alpha}(\mathbf{k})}{\partial k_x^2}. \quad (1)$$

Here and in the following we use a reduced zone scheme anticipating that the original high-temperature primitive cell doubles for a d -CDW ground state. Thus the momentum \mathbf{k} in Eq. (1) runs only over half of the high-temperature Brillouin zone whereas the index $\alpha = 1, 2$ counts the original and the backfolded electronic branches. According to Peierl's substitution rule $\chi_{\alpha}(\mathbf{k})$ are the electronic eigenstates in the normal state renormalized by many-body interaction within mean-field theory. Thus they may describe a pseudogap in the particle-hole channel but are unaffected by the superconducting gap. In our case they are given by

$$\chi_{1,2}(\mathbf{k}) = \frac{\epsilon_{\pm}(\mathbf{k})}{2} \pm \frac{1}{2} \sqrt{\epsilon_{\pm}^2(\mathbf{k}) + 4\Phi^2(\mathbf{k})}, \quad (2)$$

with $\epsilon_{\pm}(\mathbf{k}) = \epsilon(\mathbf{k}) \pm \epsilon(\mathbf{k} - \mathbf{Q})$, where $\mathbf{Q} = (\pi, \pi)$ is the wave vector of the d -CDW. $\Phi(\mathbf{k})$ is the amplitude of the d -CDW and equal to $\Phi_0 \gamma(\mathbf{k})$ with $\gamma(\mathbf{k}) = (\cos(k_x) - \cos(k_y))/2$. The bare electronic energies $\epsilon(\mathbf{k})$ are those of the t - J model in the large N limit counted from the chemical potential μ , i.e., $\epsilon(\mathbf{k}) = -2(\delta t + rJ)(\cos(k_x) + \cos(k_y)) - 4t'\delta \cos(k_x) \cos(k_y) - \mu$, with $r = 1/N_c \sum_{\mathbf{q}} \cos(q_x) f(\epsilon(\mathbf{q}))$. f is the Fermi function, δ the doping away from half-filling, J the Heisenberg coupling constant and t and t' are hopping amplitudes between nearest and next nearest neighbors on a square lattice, respectively. N_c is the original number of primitive cells. $n_{\alpha}(\mathbf{k})$ denotes the electron density with momentum \mathbf{k} and is given by

$$n_{\alpha}(\mathbf{k}) = 2T \sum_n G_{11}^{(\alpha)}(\mathbf{k}, i\omega_n) e^{i\omega_n \eta}, \quad (3)$$

where the prefactor 2 accounts for the spin degeneracy, η is an infinitesimally small positive quantity and ω_n the Matsubara frequency $(2n+1)\pi T$. $G_{11}^{(\alpha)}$ is the element (1,1) of the Green's function matrix $G^{(\alpha)}(\mathbf{k}, i\omega_n)$ defined by its inverse as,

$$G^{-1(\alpha)}(\mathbf{k}, i\omega_n) = \begin{pmatrix} i\omega_n - \chi_{\alpha}(\mathbf{k}) & -\Delta(\mathbf{k}, n) \\ -\Delta(\mathbf{k}, n) & i\omega_n + \chi_{\alpha}(\mathbf{k}) \end{pmatrix}. \quad (4)$$

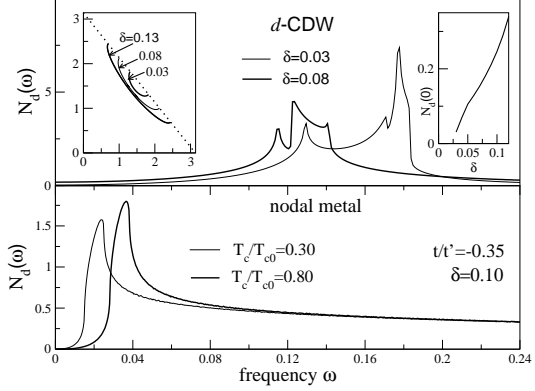


Fig. 1: D -wave projected density of states $N_d(\omega)$ in the pseudo-gap state without superconductivity for the the d -CDW (upper diagram) and the nodal metal model (lower diagram) at $T = 0$. Left and right insets show Fermi lines and $N_d(0)$, respectively, at different dopings.

The superconducting gap function $\Delta(\mathbf{k}, n)$ consists of a contribution due to the d -wave part of the Heisenberg and one due to the d -wave part of the EP interaction,

$$\Delta(\mathbf{k}, n) = -\left(\sqrt{J}\Delta_1 + \sqrt{V}\Theta(\omega_D - |\omega_n|)\Delta_3\right)\sqrt{2}\gamma(\mathbf{k}), \quad (5)$$

where Θ is the step function. In Eqs. (4)-(5) we used the fact that the phonon-induced reduction of the quasi-particle weight is independent of the ionic mass [10] and thus may be neglected in the following.

The self-consistency equation for Δ splits up into two equations for Δ_1 and Δ_3 , reading

$$(1 + F_{11})\Delta_1 + F_{12}\Delta_3 = 0, \quad (6)$$

$$F_{12}\Delta_1 + (1 + F_{22})\Delta_3 = 0, \quad (7)$$

with

$$F_{11}(\Delta_1, \Delta_3, \omega_D) = \frac{2JT}{N_c} \sum_{\mathbf{k}, n, \alpha} \frac{\gamma^2(\mathbf{k})}{(i\omega_n)^2 - \chi_{\alpha}^2(\mathbf{k}) - \Delta^2(\mathbf{k}, n)}, \quad (8)$$

$$F_{12}(\Delta_1, \Delta_3, \omega_D) = \frac{2\sqrt{JV}T}{N_c} \sum_{\mathbf{k}, n, \alpha} \frac{\gamma^2(\mathbf{k})\Theta(\omega_D - |\omega_n|)}{(i\omega_n)^2 - \chi_{\alpha}^2(\mathbf{k}) - \Delta^2(\mathbf{k}, n)}. \quad (9)$$

F_{22} is given by the expression for F_{12} if one replaces there \sqrt{JV} by V .

One important ingredient of the theory is the d -wave projected density $N_d(\omega)$ of the d -CDW model. It is shown in the upper diagram of Fig. 1 together with Fermi lines in the left inset. For the calculation we took the values $J = 0.3$ and $t' = -0.35$ measuring all energies in units of t . The right inset in Fig. 1 shows that $N_d(0)$ is nonzero

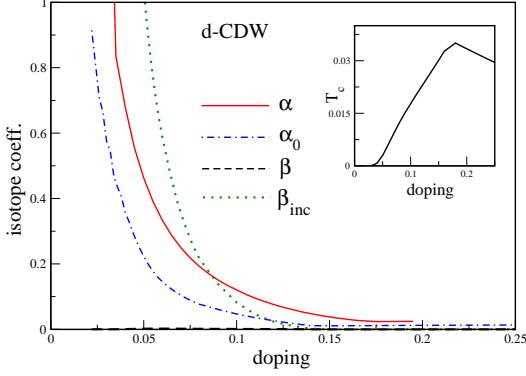


Fig. 2: (Color online) Isotope coefficients α , α_0 , β , and β_{inc} for the d -CDW model as a function of doping using $V = 0.04$ and $\omega_D = 0.16$. Inset: Suppression of T_c as a function of doping for the d -CDW model due to the evolving pseudogap. [10]

at finite δ due to finite arcs and approaches zero only in the limit $\delta \rightarrow 0$.

Recent LDA calculations [13, 14] showed that the EP interaction and in particular its d -wave part [15] is very small in cuprates. This allows to simplify Eqs.(8) and (9) by keeping only the leading terms in V . In a first step one considers $V = 0$ so that $\Delta_3 = 0$ and determines in the d -CDW case self-consistently $\Delta_1 = \bar{\Delta}_1$ and $\Phi(\mathbf{k})$ similar as in Ref. [10]. Writing then $\Delta_1 = \bar{\Delta}_1 + \Delta_2$ one may neglect F_{22} in Eq.(7) and obtains from this equation

$$\Delta_3 = -F_{12}(\bar{\Delta}_1, 0, \omega_D)\bar{\Delta}_1. \quad (10)$$

Eq.(8) yields, again in leading order in V ,

$$\Delta_2 = \left(F_{12}^2(\bar{\Delta}_1, 0, \omega_D) - \Delta_3 \frac{\partial F_{11}(\bar{\Delta}_1, \Delta_3, \omega_D)}{\partial \Delta_3} \right) / \frac{\partial F_{11}(\Delta_1, 0, \omega_D)}{\partial \Delta_1}. \quad (11)$$

After taking the derivatives in Eq. (11) Δ_1 and Δ_3 should be put to $\bar{\Delta}_1$ and 0, respectively. Assuming that Λ depends on ω_D only via Δ_1 and Δ_3 and noting that Eqs. (10) and (11) hold for a general ω_D one may easily form the derivatives of Δ_2 and Δ_3 with respect to ω_D and thus obtain β .

In principle there are two more sources for a dependence of Λ on M : The bare one-particle energies $\epsilon(\mathbf{k})$ may depend on M . Such a case may occur if the EP interaction can no longer be described by Eliashberg theory because strong polaronic or non-adiabatic effects play an important role. However, there is overwhelming evidence, both from experiment [16] and theory [13, 14], that this is not the case. For instance, recent angle resolved photoemission (ARPES) experiments on nearly optimally doped Bi2212 [16] show that the band width does not change within the experimental error when substituting O^{16} by O^{18} . Using the polaronic model [17] an observed value of

$\beta \sim 1$ would require a 12 per cent change of the electronic band width which is not observed. Another possibility for a M dependence of Λ could be due to the d -CDW gap $\Phi(\mathbf{k})$. Recently we have shown [10] that the onset temperature T^* for the d -CDW gap shows practically no isotope effect which should also hold for the $T = 0$ d -CDW gap $\Phi(\mathbf{k})$.

Numerical results for the isotope coefficients α , α_0 , and β , which are related to T_c , the $T = 0$ superconducting gap and the phase stiffness, respectively, are shown in Fig. 2 for the d -CDW model. The calculation of α has been described previously [10], α_0 is defined by

$$\alpha_0 = \frac{\omega_D}{2\Delta_1} \frac{\partial \Delta_1}{\partial \omega_D}. \quad (12)$$

Outside of the pseudogap state, i.e., for $\delta \geq \delta_c \sim 0.145$, all three coefficients are very small. Here α and α_0 are much smaller than the BCS value of $1/2$ because superconductivity is mainly determined by J and not by V because of the small employed value for V . Entering the pseudogap state α and α_0 nevertheless increase strongly with decreasing doping due to the evolving pseudogap as explained in detail in Ref. [10]. In contrast to that β does not change much below δ_c and remains practically zero throughout the underdoped region. Considering only the underdoped region, i.e., $\delta \leq \delta_c$, one could also use the ratio T_c/T_{c0} as an independent variable instead of δ . The curves in Fig. 2 would not look much different in such a plot because T_c depends rather linearly on δ in that region, as shown in the inset of Fig. 2.

To understand the surprising behavior of β we present now approximate analytic expressions for β and various other quantities which become asymptotically exact at small values of the superconducting gap but are also rather accurate over the whole doping region. Evaluating Eq.(1) for an infinite cutoff and neglecting momentum derivatives of the order parameter we find

$$\Lambda = \frac{1}{2N_c} \sum_{\mathbf{k}, \alpha} \frac{\Delta^2(\mathbf{k})(\nabla \chi_\alpha(\mathbf{k}))^2}{E_\alpha^3(\mathbf{k})}, \quad (13)$$

and

$$X = \left(\frac{\beta}{\alpha_0} + 1 \right) \frac{\Lambda}{3} = \frac{1}{2N_c} \sum_{\mathbf{k}, \alpha} \frac{\Delta^2(\mathbf{k})\chi_\alpha^2(\mathbf{k})(\nabla \chi_\alpha(\mathbf{k}))^2}{E_\alpha^5(\mathbf{k})}. \quad (14)$$

The main contribution in the sums over momentum in Eqs.(13) and (14) comes from the region near the arcs which consists of all points $\{\mathbf{k}_{F\alpha}\}$ satisfying $\chi(\mathbf{k}_{F\alpha}) = 0$. Correspondingly, we split these sums into a part parallel and a part perpendicular to the arcs. Assuming that the electron dispersion perpendicular to the arcs can be approximated linearly we find that the integrations perpendicular to the arcs diverge for small $\Delta(\mathbf{k})$ cancelling, for instance, the prefactor $\Delta^2(\mathbf{k})$ in Eq.(13). The remaining integration parallel to the arcs in Λ and X can be written

as surface integrals along the arcs yielding

$$\Lambda = \sum_{\alpha} \oint \frac{dS(\mathbf{k}_{F\alpha})}{4\pi^2 v(\mathbf{k}_{F\alpha})} (\nabla \chi_{\alpha}(\mathbf{k}_{F\alpha}))^2, \quad (15)$$

and $X = \Lambda/3$, or equivalently,

$$\beta/\alpha_0 = 0. \quad (16)$$

Eq.(16) explains the tiny values for β in Fig. 2 obtained by numerical evaluation of the exact expressions for β . The small values for β throughout the underdoped region reflect directly the divergencies encountered in the momentum integrations perpendicular to the arcs. If there would be no divergencies the right-hand side of Eq.(14) would smoothly approach the right-hand side of Eq.(13) for $\Delta(\mathbf{k}) \rightarrow 0$. Thus we would obtain $\beta/\alpha_0 = 2$ and an increasing β towards small dopings both of which would be in excellent agreement with experiment. This suggests that the above mentioned divergencies actually do not occur in the high- T_c superconductors so far studied with respect to β .

One model which has a pseudogap but no arcs and thus no divergencies in momentum sums is the nodal metal (NM) model [3,9]. Its dispersion is given by

$$\chi_{1,2}(\mathbf{k}) = \pm \sqrt{\epsilon^2(\mathbf{k}) + \Phi^2(\mathbf{k})}, \quad (17)$$

which formally can be obtained from Eq. (2) by putting $\epsilon_+(\mathbf{k}) = 0$. The NM model does not allow to determine Φ_0 but considers it as a parameter. Following Ref. [9] it is convenient not to use Φ_0 as an independent variable but the ratio T_c/T_{c0} which describes the reduction of T_c due to $\Phi(\mathbf{k})$ relative to the maximum transition temperature T_{c0} at $\delta = \delta_c$. Dependencies on T_c/T_{c0} may be interpreted as doping dependencies due to the monotonic relation between T_c and δ in the underdoped region, see the inset of Fig. 2 in case of the d -CDW system. The lower diagram in Fig. 1 shows $N_d(\omega)$ for the NM model for $\delta = 0.10$ and two values for T_c/T_{c0} . $N_d(0)$ is zero in all cases because of the absence of arcs.

The calculation of β proceeds in the same way as for the d -CDW model. Fig. 3 shows numerical results for α , α_0 , β , and the ratio β/α_0 using $V = 0.04$ and $\omega_D = 0.16$. Unlike in Fig. 2 β increases strongly with decreasing T_c/T_{c0} and the ratio β/α_0 is near two over a large part of the underdoped region, approaching exactly 2 for $T_c/T_{c0} \rightarrow 0$. Since α and α_0 are of similar magnitude this implies also $\beta/\alpha \sim 2$ which is exactly the value found in experiment. The diagram also shows that β assumes values of 1 and larger already for moderate reductions in T_c . This is rather astonishing because it means that the small EP coupling constant found in LDA calculations [13–15] is able to produce the large value for β of Fig. 3. Varying the Debye frequency over a large frequency region does not change much the curves in Fig. 2 and Fig. 3. Similar as in the case of α discussed in Ref. [10] α_0 and β do not show anomalies if the phonon frequency and the pseudogap are

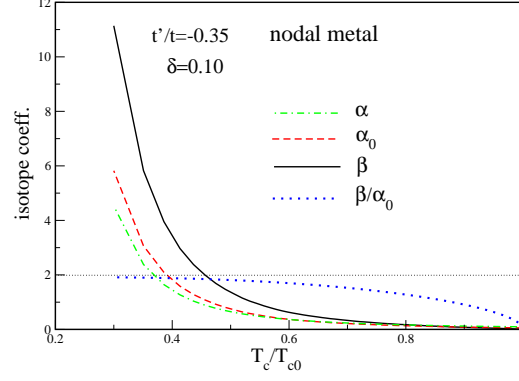


Fig. 3: (Color online) Isotope coefficients α , α_0 , β and the ratio β/α_0 for the nodal metal model as a function of T_c/T_{c0} for a fixed doping $\delta = 0.10$ using $V = 0.04$ and $\omega_D = 0.16$.

close to each other. Actually, for all phonon frequencies smaller than about 0.16 the pseudogap crosses the phonon at some doping without any effect on the curves showing that the large increases in the underdoped region are not due to resonance effects between the phonon and the pseudogap.

Important details of Fig. 3 such as the behavior of the ratio β/α_0 can be understood again by an approximate analytic evaluation of the sums over momenta. Since the NM model has no arcs one may expand $\epsilon(\mathbf{k})$ around the high-temperature Fermi line given by $\epsilon(\mathbf{k}) = 0$. Splitting again the momenta sums into perpendicular and parallel parts, taking $\Phi(\mathbf{k})$ right on the Fermi line and linearising $\epsilon(\mathbf{k})$ the integration perpendicular to the Fermi line can be carried out and is always finite. As a result β and X can again be written as surface integrals. Due to the absence of divergencies $X \rightarrow \Lambda$ for $\Delta(\mathbf{k}) \rightarrow 0$ yielding $\beta/\alpha_0 \rightarrow 2$. This result is rather general and just expresses the absence of divergencies.

Many features of the NM model agree with the experiment, for instance, the observed ratio $\beta/\alpha \sim 2$ over most of the underdoped region and the large increase of α and β with decreasing T_c . Obviously it has also short-comings. For instance, the lower diagram of Fig. 1 implies a pseudogap of only about 0.02 or 10 meV for a decrease T_c/T_{c0} of 0.3 which is unrealistically small. The more fundamental question, however, is whether this model with perfect nesting in the particle-hole channel is applicable to the cuprates at all. ARPES experiments in extremely underdoped Bi2212 [18] found an excitation spectrum of the pseudogap phase without superconductivity which is very similar to the NM model. These data, however, have been interpreted in terms of a superconducting order parameter with finite phase correlation length. Since superconductivity does not renormalize the one-electron spectrum entering the phase stiffness the resulting β would be equally small as in a superconductor without pseudogap and thus disagree with experiment. Nodal metal behavior can, how-

ever, be realized to some extent for an incommensurate d -CDW state. The nesting condition $\epsilon_+(\mathbf{k}) = 0$ of the NM model can in this case be fulfilled in limited regions around \mathbf{k} points on Fermi lines which are connected by nesting vectors and exhibit parallel tangents to the Fermi line. Assuming four nesting vectors of the form $\mathbf{Q} = (\pi, \pi \pm \delta_{inc})$ and $(\pi \pm \delta_{inc}, \pi)$, determining δ_{inc} from the nesting condition and correlating only pairs of states with maximal nesting we obtained the dotted line β_{inc} in Fig. 2 for β . It shows the desired increase towards low doping but the calculated ratio $\beta_{inc}/\alpha_{0,inc}$ (not shown in Fig. 2) deviates substantially from 2 due to divergencies at Fermi lines near the antinodal point. It also has been shown [19] that superconductivity (not taken into account above in determining δ_{inc}) suppresses δ_{inc} strongly, suggesting that incommensurability is not causal for the large observed values for β .

The above results show that the presence of arcs (or, more general, a finite length of the Fermi line) at $T = 0$ in the pseudogap state (i.e., without superconductivity) are generically incompatible with large values of β in the underdoped region. This holds for all models where the pseudogap phase has long-range order and arises in the particle-hole channel which necessarily leads to arcs in two-dimensional models due to imperfect nesting. The d -CDW model is one example. It also holds for short-range models [20] for the pseudogap which are Fermi liquids, i.e., where the self-energy at $T = 0$ can be expanded in powers of the momentum and frequency. In this case the arcs are nothing else than the Fermi lines in the normal state without pseudogap and the arguments used above for Fermi arcs apply. Large values for β can therefore only be expected if no arcs exist at all as in the NM model or that the divergencies in the integration perpendicular to the arcs in calculating β are not present for some reason. One possibility could be a non-Fermi liquid ground state without infinitely sharp quasiparticles and a broad spectral function.

In conclusion we have investigated the isotope coefficient β of the magnetic penetration depth at $T = 0$ using two models for the pseudogap. The calculation shows that β depends severely on the presence or absence of Fermi arcs at $T = 0$ in the absence of superconductivity. The experimentally observed large increase of β in the underdoped region is reproduced in the case of a nodal metal using a small EP coupling consistent with first-principles calculations based on the local density approximation. The d -CDW model is generic for models with two competing order parameters often used to interpret experimental results. [21,22] The resulting β , however, is small throughout the underdoped region and disagrees with experiment even if the EP coupling constant is increased by orders of magnitude. Responsible for the absence of an enhancement of β is the presence of Fermi arcs which lead to divergent \mathbf{k} integrals perpendicular to the arcs in calculating β . We hope that the discovered link between arcs and the isotope coefficient β motivates more experimental work on

the doping dependence of β .

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